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# 2-Benzoylpyridine Ligand Complexation with Gold Critical for Propargyl Ester-Based Protein Labeling

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## Abstract

© 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim In previously reported work, AuIIIcomplexes coordinated with 2-benzoylpyridine ligand, BPy-Au, were prebound to a protein and used to discover a novel protein-directed labeling approach with propargyl ester functional groups. In this work, further examination discovered that gold catalysts devoid of the 2-benzoylpyridine ligand (e.g., NaAuCl4) had significantly reduced levels of protein labeling. Mechanistic investigations then revealed that BPy-Au and propargyl esters undergo a rare example of C(sp2)−C(sp) aryl–alkynyl cross-coupling, likely through spontaneous reductive elimination. Overall, these observations appear to suggest that BPy-Au-mediated, propargyl ester-based protein labeling acts via an activated ester intermediate, which contributes to our understanding of this process and will aid the expansion/optimization of gold-catalyst usage in future bioconjugation applications, especially in vivo.

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## Keywords

alkynes, amides, cross coupling, gold catalysis, protein conjugation

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